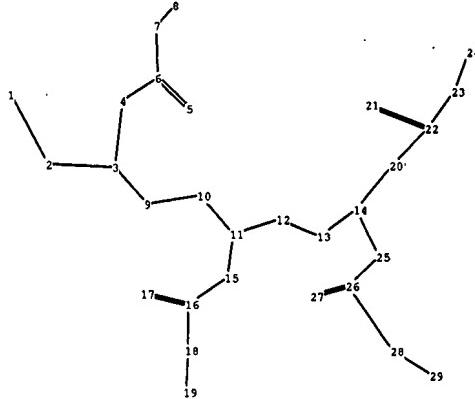
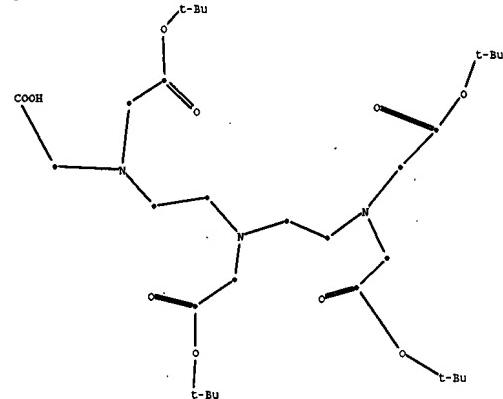


EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	3219	"424/184.1".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:17
L2	868	"530/403".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:17
L3	853	"560/41".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:18
L4	133	((WILLIAM) near2 (MCBRIDE)). INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:18
L5	150	((DAVID) near2 (GOLDENBERG)). INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:18
L6	42	((WILLIAM) near2 (MCBRIDE)). INV.	EPO; JPO; DERWENT	OR	ON	2007/10/29 16:18
L7	84	((DAVID) near2 (GOLDENBERG)). INV.	EPO; JPO; DERWENT	OR	ON	2007/10/29 16:19
L10	583	L2 AND @AY<"1998"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:21
L11	1030	L1 AND @AY<"1998"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:21
L12	404	L3 AND @AY<"1998"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/29 16:26
L13	4	("6962702") or ("7074405") or ("7138103") or ("7052872").PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2007/10/29 16:59
L14	4	(("5695737") or ("6080785") or ("6607710") or ("7052872") or ("2006264669")).PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2007/10/29 17:02
L15	5	(("5695737") or ("6080785") or ("6607710") or ("7052872") or ("20060264669")).PN.	US-PGPUB; USPAT; USOCR	OR	OFF	2007/10/29 17:02
L16	2	("6080785").URPN.	USPAT	OR	ON	2007/10/29 17:03



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28
29

chain bonds :

1-2 2-3 3-4 3-9 4-6 5-6 6-7 7-8 9-10 10-11 11-12 11-15 12-13 13-14 14-20 14-25 15-16
16-17 16-18 18-19 20-22 21-22 22-23 23-24 25-26 26-27 26-28 28-29

exact/norm bonds :

2-3 3-4 3-9 5-6 6-7 10-11 11-12 11-15 13-14 14-20 14-25 16-17 16-18 21-22 22-23 26-27
26-28

exact bonds :

1-2 4-6 7-8 9-10 12-13 15-16 18-19 20-22 23-24 25-26 28-29

Match level :

1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS
12:CLASS13:CLASS14:CLASS15:CLASS16:CLASS17:CLASS18:CLASS19:CLASS20:CLASS21:CLASS
22:CLASS23:CLASS24:CLASS25:CLASS26:CLASS27:CLASS28:CLASS29:CLASS

10/776470 Therapeutic n DiagnosticConjugates

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NEWS 2 JUL 02 LMEDLINE coverage updated
NEWS 3 JUL 02 SCISEARCH enhanced with complete author names
NEWS 4 JUL 02 CHEMCATS accession numbers revised
NEWS 5 JUL 02 CA/CAplus enhanced with utility model patents from China
NEWS 6 JUL 16 CAplus enhanced with French and German abstracts
NEWS 7 JUL 18 CA/CAplus patent coverage enhanced
NEWS 8 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9 JUL 30 USGENE now available on STN
NEWS 10 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 11 AUG 06 FSTA enhanced with new thesaurus edition
NEWS 12 AUG 13 CA/CAplus enhanced with additional kind codes for granted patents
NEWS 13 AUG 20 CA/CAplus enhanced with CAS indexing in pre-1907 records
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NEWS 16 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 17 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 18 SEP 13 FORIS renamed to SOFIS
NEWS 19 SEP 13 INPADOCDB enhanced with monthly SDI frequency
NEWS 20 SEP 17 CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 21 SEP 17 CAplus coverage extended to include traditional medicine patents
NEWS 22 SEP 24 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 23 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 24 OCT 19 BEILSTEIN updated with new compounds

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

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=>
Uploading C:\Program Files\Stnexp\Queries\2007 cases\10766470\molecule V c1118.str

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 16:56:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -          14 TO ITERATE
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100.0% PROCESSED 14 ITERATIONS
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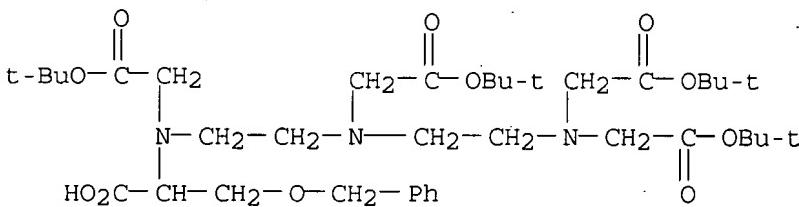
1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 56 TO 504
 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d sca

L2 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 2-Oxa-5,8,11-triazatridecan-13-oic acid, 4-carboxy-5,8,11-tris[2-(1,1-dimethylethoxy)-2-oxoethyl]-1-phenyl-, 13-(1,1-dimethylethyl) ester (9CI)
 MF C38 H63 N3 O11



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 11 sss full
 FULL SEARCH INITIATED 16:56:50 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 287 TO ITERATE

100.0% PROCESSED 287 ITERATIONS
 SEARCH TIME: 00.00.01

5 ANSWERS

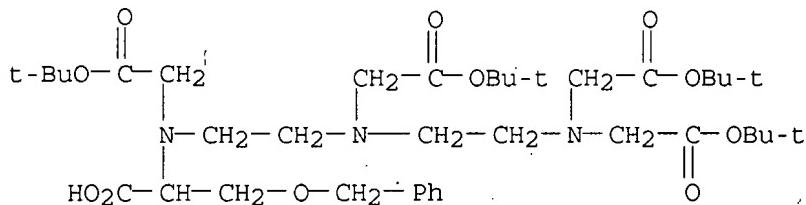
L3 5 SEA SSS FUL L1

=> d sca str rn
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=> d sca

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 2-Oxa-5,8,11-triazatridecan-13-oic acid, 4-carboxy-5,8,11-tris[2-(1,1-dimethylethoxy)-2-oxoethyl]-1-phenyl-, 13-(1,1-dimethylethyl) ester (9CI)
 MF C38 H63 N3 O11

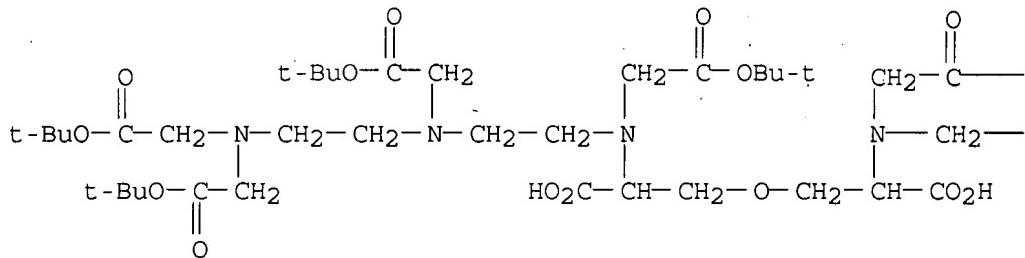


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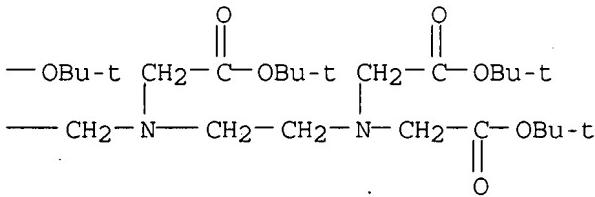
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1) :5

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
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 2,5,8,14,17,20-hexakis[2-(1,1-dimethylethoxy)-2-oxoethyl]-,
 1,21-bis(1,1-dimethylethyl) ester (9CI)
MF C62 H112 N6 O21

PAGE 1-A

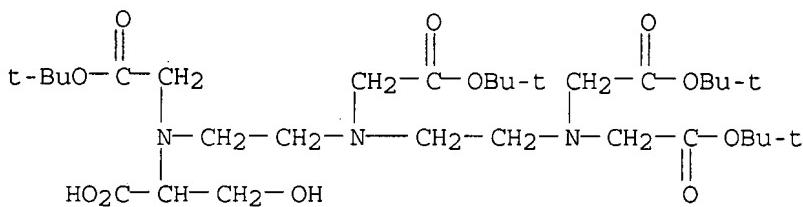


PAGE 1-B



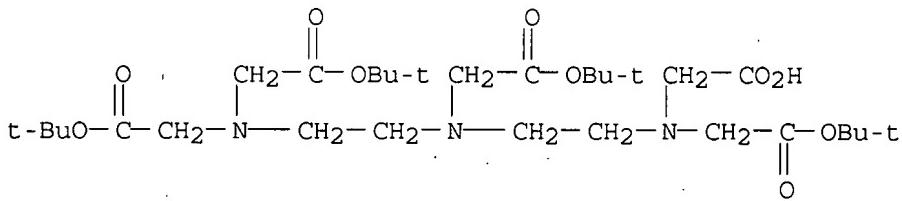
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 3-Oxa-6,9,12-triazatetradecan-14-oic acid, 6-(1-carboxy-2-hydroxyethyl)-
9,12-bis[2-(1,1-dimethylethoxy)-2-oxoethyl]-2,2-dimethyl-4-oxo-,
14-(1,1-dimethylethyl) ester (9CI)
MF C31 H57 N3 O11



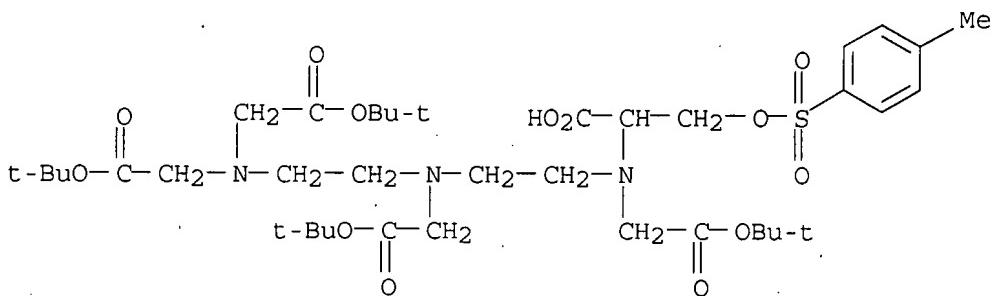
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
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 MF C30 H55 N3 O10



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 3-Oxa-6,9,12-triazatetradecan-14-oic acid, 6-[1-carboxy-2-[(4-methylphenyl)sulfonyloxy]ethyl]-9,12-bis[2-(1,1-dimethylethoxy)-2-oxoethyl]-2,2-dimethyl-4-oxo-, 14-(1,1-dimethylethyl) ester (9CI)
 MF C38 H63 N3 O13 S



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ALL ANSWERS HAVE BEEN SCANNED

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| L2 | 1 S L1 |
| L3 | 5 S L1 SSS FULL |

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=> s 13
L4 20 L3

=> d 13 1-20 ibib abs
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=> d 14 1-20 ibib abs

L4 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1224889 HCAPLUS
DOCUMENT NUMBER: 145:505757
TITLE: Method for manufacturing diethylenetriaminepentaacetic acid derivatives

10/776470 Therapeutic n DiagnosticConjugates

INVENTOR(S) : Lee, Te-Wei; Yang, Chia-Hsi; Ho, Yen-Sheng; Lu, Li-Hui; Chen, Shu-Ling
PATENT ASSIGNEE(S) : Atomic Energy Council - Institute of Nuclear Energy Research, Taiwan
SOURCE: U.S. Pat. Appl. Publ., 10pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------------------|------|----------|-----------------|------------|
| US 2006264669 | A1 | 20061123 | US 2005-134397 | 20050523 |
| JP 2006342105 | A | 20061221 | JP 2005-169511 | 20050609 |
| PRIORITY APPLN. INFO. : | | | US 2005-134397 | A 20050523 |

OTHER SOURCE(S) : MARPAT 145:505757

AB The invention relates to regioselective hydrolysis of diethylenetriaminepentaacetic acid (DTPA) tetraalkyl esters by using a metal ion as catalyst to obtain monoreactive DTPA tetraalkyl esters. Thus, DTPA pentaethyl ester (prepared from DTPA dianhydride) in aqueous NaOH solution containing CuCl₂ was bubbled with H₂S and the solution filtered to remove Cu₂S to yield 61 % DTPA tetra-Et ester in which the free carboxy group is at the terminal position.

L4 ANSWER 2 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:495678 HCPLUS
DOCUMENT NUMBER: 145:140459
TITLE: Phosphorylation State-Responsive Lanthanide Peptide Conjugates: A Luminescence Switch Based on Reversible Complex Reorganization

AUTHOR(S) : Tremblay, Matthew S.; Zhu, Qing; Marti, Angel A.; Dyer, Joanne; Halim, Marlin; Jockusch, Steffen; Turro, Nicholas J.; Sames, Dalibor

CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA

SOURCE: Organic Letters (2006), 8(13), 2723-2726
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S) : CASREACT 145:140459

AB A luminogenic probe for peptide dephosphorylation has been developed. It consists of a serine-/tyrosine-containing peptide modified on the N-terminus with a tryptophan residue and a DTPA chelate capable of binding Tb³⁺. The authors propose a mechanistic model for the luminescence enhancement based on the interconversion of monomeric and dimeric lanthanide species, which is affected by the phosphorylation state of the serine or tyrosine residue. The optical switch reports effectively on phosphatase-catalyzed dephosphorylation in vitro.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:487757 HCPLUS
DOCUMENT NUMBER: 146:402266
TITLE: Development of a ¹¹¹In-labeled peptide derivative

targeting a chemokine receptor, CXCR4, for imaging tumors
AUTHOR(S) : Hanaoka, Hirofumi; Mukai, Takahiro; Tamamura, Hirokazu; Mori, Tomohiko; Ishino, Seigo; Ogawa, Kazuma; Iida, Yasuhiko; Doi, Ryuichiro; Fujii, Nobutaka; Saji, Hideo
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Kyoto University, Yoshida Shimoadaichi-cho, Sakyo-ku, Kyoto, 606-8501, Japan
SOURCE: Nuclear Medicine and Biology (2006), 33(4), 489-494
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The chemokine receptor CXCR4 is highly expressed in tumor cells and plays an important role in tumor metastasis. The aim of this study was to develop a radiopharmaceutical for the imaging of CXCR4-expressing tumors *in vivo*. Based on structure-activity relationships, the authors designed a 14-residue peptidic CXCR4 inhibitor, Ac-TZ14011, as a precursor for radiolabeled peptides. For ¹¹¹In-labeling, diethylenetriaminepentaacetic acid (DTPA) was attached to the side chain of D-Lys8 which is distant from the residues indispensable for the antagonistic activity. In-DTPA-Ac-TZ14011 inhibited the binding of a natural ligand, stromal cell-derived factor-1 α , to CXCR4 in a concentration-dependent manner with IC₅₀ = 7.9 nM (Ac-TZ14011: 1.2 nM). In biodistribution expts., more ¹¹¹In-DTPA-Ac-TZ14011 accumulated in the CXCR4-expressing tumor than in blood or muscle. Furthermore, the tumor-to-blood and tumor-to-muscle ratios were significantly reduced by coinjection of Ac-TZ14011, indicating a CXCR4-mediated accumulation in tumor. These findings suggested that ¹¹¹In-DTPA-Ac-TZ14011 would be a potential agent for the imaging of CXCR4 expression in metastatic tumors *in vivo*.
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:951424 HCAPLUS
DOCUMENT NUMBER: 143:422550
TITLE: Synthesis of DTPA-conjugated (1,4)-linked 2-amino-glycosides varying in the anomeric configuration and their MRI contrast effect
AUTHOR(S) : Tanaka, Hiroshi; Ando, Yoshio; Wada, Masatoshi; Takahashi, Takashi
CORPORATE SOURCE: Department of Applied Chemistry, Graduate School of Science and Engineering, Tokyo Institute of Technology, Tokyo, Meguro, 152-8552, Japan
SOURCE: Organic & Biomolecular Chemistry (2005), 3(18), 3311-3328
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The efficient synthesis of diethylenetriamine-N,N,N',N'',N'''-penta-acetic acid (DTPA)-conjugated oligosaccharides composed of α - and/or β -linked tri to mono-glucosamines is described. Gd(III) complex with DTPA-conjugated chitotriitol has been reported to be an effective MRI contrast agent. In order to elucidate the structure-property relationships, we planned to synthesize the DTPA-conjugated 2-amino-tri-, di-, and monosaccharides varying in configuration at the anomeric

positions and the C2 position on the reducing end. Our strategy for the synthesis of the DTPA-conjugated oligosaccharides involves O-per-benzyl protected 2-amino-tri-, di-, and monosaccharides as key intermediates. The 2-amino-glycosides were prepared by non-selective glycosidation of 2-azido-2-deoxy-glycosyl donors, followed by separation of two anomeric isomers. Although the synthesis involves separation of the stereoisomers, it circumvents not only the careful tuning of reaction conditions, but also the time-consuming preparation of glycosyl donors attached to different protecting groups. The protected 2-amino-glycosides were converted to the fully deprotected DTPA-conjugated tri- to monosaccharides by the same operation. MRI phantom study using the Gd(III) complexes of DTPA-conjugated oligosaccharides indicates that the number of the monosaccharide units was critical for enhancing the relative signal intensity of water protons per Gd, and various stereoisomers would be candidate scaffolds for MRI contrast agents.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:235070 HCAPLUS
 DOCUMENT NUMBER: 142:293787
 TITLE: Somatostatin analogs and metal complexes for MRI diagnosis and treatment of tumors
 INVENTOR(S): Saito, Hiroshi; Saji, Hideo; Arano, Yasushi; Iwafuchi, Akimasa; Mifune, Masaki; Mukai, Takahiro; Akisawa, Hiroyuki; Takimoto, Yamato
 PATENT ASSIGNEE(S): Nihon Mediphysics Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| JP 2005068046 | A | 20050317 | JP 2003-297606 | 20030821 |
| PRIORITY APPLN. INFO.: | | | JP 2003-297606 | 20030821 |
| OTHER SOURCE(S): | MARPAT | 142:293787 | | |

AB Somatostatin analogs (I, RNHCH(CH₂X)CO-Cys-A-dTrp-Lys-B-Cys-Y wherein R = chelator residue, including DTPA, DOTA, etc.; X = carboxyl, aminophenyl, naphthyl; Y = Thr-OH, Thr-NH₂, Trp-NH₂; A = Phe, Tyr; B = Thr, Val) and metal complexes are claimed for MRI diagnosis and treatment of tumors by targeting somatostatin receptors. ¹¹¹In complexes were prepared, and their pharmacokinetics in tissues were determined

L4 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:15791 HCAPLUS
 DOCUMENT NUMBER: 142:120462
 TITLE: Therapeutic and diagnostic conjugates for use with multispecific antibodies
 INVENTOR(S): McBride, William J.; Goldenberg, David M.; Noren, Carl; Hansen, Hans J.
 PATENT ASSIGNEE(S): Immunomedics, Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 53 pp., Cont.-in-part of U.S. Ser. No. 150,654.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 19

PATENT INFORMATION:

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| US 2005002945 | A1 | 20050106 | US 2004-776470 | 20040211 |
| US 7074405 | B1 | 20060711 | US 1999-337756 | 19990622 |
| US 7052872 | B1 | 20060530 | US 1999-382186 | 19990823 |
| US 2002006379 | A1 | 20020117 | US 2001-823746 | 20010403 |
| US 6962702 | B2 | 20051108 | | |
| US 2003198595 | A1 | 20031023 | US 2002-150654 | 20020517 |
| US 7138103 | B2 | 20061121 | | |
| AU 2005211754 | A1 | 20050825 | AU 2005-211754 | 20050211 |
| CA 2555666 | A1 | 20050825 | CA 2005-2555666 | 20050211 |
| WO 2005077071 | A2 | 20050825 | WO 2005-US4177 | 20050211 |
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TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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| EP 1720575 | A2 | 20061115 | EP 2005-726492 | 20050211 |
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| JP 2007528372 | T | 20071011 | JP 2006-553216 | 20050211 |
| PRIORITY APPLN. INFO.: | | | US 1998-90142P | P 19980622 |
| | | | US 1998-104156P | P 19981014 |
| | | | US 1999-337756 | A2 19990622 |
| | | | US 1999-382186 | B2 19990823 |
| | | | US 2001-823746 | A2 20010403 |
| | | | US 2002-150654 | A2 20020517 |
| | | | US 2004-776470 | A 20040211 |
| | | | WO 2005-US4177 | W 20050211 |

OTHER SOURCE(S): MARPAT 142:120462

AB Disclosed are compds. that include two or more haptens conjugated by a spacer or a carrier. The haptens may include diethylenetriaminepentaacetate (DTPA), histamine-succinyl-glutamine (HSG), or combinations of DTPA and HSG. The compds. also includes an effector mol. which may be conjugated to one or more of the haptens, the spacer/carrier, or both. The effector mol. may be conjugated by a number of linkages including an ester linkage, an imino linkage, an amino linkage, a sulfide linkage, a thiosemicarbazone linkage, a semicarbazone linkage, an oxime linkage, an ether linkage, or combinations of these linkages. Also disclosed are methods of synthesizing the compds. and/or precursors of the compds.

L4 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:795339 HCAPLUS

DOCUMENT NUMBER: 141:421892

TITLE: De Novo Designed Peptidic Redox Potential Probe:
Linking Sensitized Emission to Disulfide Bond

10/776470 Therapeutic n DiagnosticConjugates

AUTHOR(S): Formation
Lee, Kyung; Dzubeck, Valerie; Latshaw, Lauren;
Schneider, Joel P.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University
of Delaware, Newark, DE, 19716-2522, USA

SOURCE: Journal of the American Chemical Society (2004),
126(42), 13616-13617

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:421892

AB The design and utility of a peptidic probe capable of accurately measuring environmental redox potential via sensitized emission has been prepared. This probe is characterized by long-lived luminescence (millisecond), nanomolar detection limits, and a probe reduction potential of -0.243 V.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:144091 HCPLUS
DOCUMENT NUMBER: 141:391077

TITLE: Effect of carboxylation of N-terminal phenylalanine of 111In-DTPA (diethylenetriaminepentaacetic acid)-octreotide on accumulation of radioactivity in kidney

AUTHOR(S): Akizawa, Hiromichi; Takimoto, Hirokazu; Saito, Madoka; Iwado, Akimasa; Mifune, Masaki; Saito, Yutaka; Uehara, Tomoya; Arano, Yasushi; Mukai, Takahiro; Hanaoka, Hirofumi; Saji, Hideo

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Okayama University, Okayama, 700-8530, Japan

SOURCE: Biological & Pharmaceutical Bulletin (2004), 27(2), 271-272

CODEN: BPBLEO; ISSN: 0918-6158

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB For purpose of reducing renal accumulation of radioactivity of a known radiopharmaceutical agent, i.e., 111In-DTPA (diethylenetriaminepentaacetic acid)-D-Phel-octreotide, a derivative in which p-carboxy-L-phenylalanine is substituted for D-Phel was synthesized. Biodistribution study of the resultant compound having carboxy-substituted L-Phel revealed that the renal accumulation was significantly lower than that of control compound having unsubstituted L-Phel, demonstrating that the presence of neg. charge on the N-terminal amino acid of octreotide is effective to reduce the renal accumulation. This effect can be attributed to the reduction of lipophilicity and also the repulsive force arisen from the neg. charge of renal brush border membrane.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:959352 HCPLUS
DOCUMENT NUMBER: 138:142331

TITLE: Design, Synthesis, and Evaluation of Gadolinium Cationic Lipids As Tools for Biodistribution Studies of Gene Delivery Complexes

AUTHOR(S): Leclercq, Francoise; Cohen-Ohana, Mirit; Mignet, Nathalie; Sbarbati, Andrea; Herscovici, Jean; Scherman, Daniel; Byk, Gerardo

CORPORATE SOURCE: Department of Chemistry, Laboratory of Peptidomimetics and Genetic Chemistry, Bar Ilan University, Ramat Gan, 52900, Israel

SOURCE: Bioconjugate Chemistry (2003), 14(1), 112-119
CODEN: BCCHE; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Gadolinium-chelating cationic lipids have been synthesized to obtain lipoplexes with MRI contrast properties. These compds. were designed to follow the biodistribution of synthetic DNA for gene delivery by NMR imaging. The lipid MCO-I-68 was synthesized, and chelate complexes with gadolinium were formed and characterized in terms of physicochem. and DNA binding properties. The transfection activity of MCO-I-68-Gd/DNA complexes was assayed in vitro on NIH 3T3. Different formulations of the product were tested. When up to 5% of the gadolinium lipid complexes were co-formulated with the cationic lipid RPR120535 used as a reference, the transfection levels were maintained as compared to RPR120535 alone. To date, only a liposomal formulation of a gadolinium-cationic lipid chelate without DNA had been observed using magnetic resonance imaging. In vivo intratumoral administration of MCO-I-68-Gd/DNA lipoplexes to tumor model led to an important increase of the NMR signal. It was demonstrated that the new complexes also acted as transfection carriers when they were formulated from liposomes.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:407215 HCPLUS
DOCUMENT NUMBER: 136:81993
TITLE: Significance of ¹¹¹In-DTPA chelate in renal radioactivity levels of ¹¹¹In-DTPA-conjugated peptides
AUTHOR(S): Akizawa, H.; Arano, Y.; Mifune, M.; Iwado, A.; Saito, Y.; Uehara, T.; Ono, M.; Fujioka, Y.; Ogawa, K.; Kiso, Y.; Saji, H.
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Okayama University, Tsushima-naka, Okayama, 700-8530, Japan
SOURCE: Nuclear Medicine and Biology (2001), 28(4), 459-468
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Metabolic studies of ¹¹¹In-DTPA-labeled polypeptides and peptides showed that the radiolabeled (poly)peptides generated ¹¹¹In-DTPA-adducts of amino acid that possess long residence times in the lysosomal compartment of the tissues where (poly)peptides accumulated. However, a recent study suggested that metal-chelate-methionine (Met) might possess in vivo behaviors different from metal-chelate adducts of other amino acids. In this study, to elucidate whether some biol. characteristics of Met may accelerate the renal elimination rate of ¹¹¹In-DTPA-adduct of Met into urine, ¹¹¹In-DTPA-Met1-octreotide was synthesized and the renal handling of ¹¹¹In-DTPA-Met was investigated using ¹¹¹In-DTPA-1-Phe1-octreotide (Phe represents phenylalanine), which was reported previously, as a reference. Both ¹¹¹In-DTPA-conjugated octreotide analogs were stable against 3-h incubation in murine serum at 37°C. Both ¹¹¹In-DTPA-octreotide

analogs also showed rapid clearance of the radioactivity from the blood and similar accumulation of the radioactivity in the kidney. No significant differences were observed in the renal radioactivity levels from 10 min to 24 h postinjection between the two. Metabolic studies indicated that ¹¹¹In-DTPA-Met1-octreotide and ¹¹¹In-DTPA-1-Phe1-octreotide generated ¹¹¹In-DTPA-adducts of Met and Phe, resp., as the final radiometabolites at similar rates. These findings suggested that the long residence times of the radioactivity in tissues after administration of ¹¹¹In-DTPA-labeled peptides and polypeptides would be attributed to inherent characteristics of ¹¹¹In-DTPA chelate.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:279459 HCPLUS
 DOCUMENT NUMBER: 134:292147
 TITLE: Bisphosphonic acid derivative and compound thereof labelled with radioactive nuclide
 INVENTOR(S): Ito, Osamu; Kanazashi, Nobuhiko; Morishita, Aki; Hara, Masamichi; Kanagawa, Masaru; Watanabe, Yasuko; Itaya, Yoshitoshi
 PATENT ASSIGNEE(S): Nihon Medi-Physics Co., Ltd., Japan
 SOURCE: Eur. Pat. Appl., 24 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English.
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|------------|
| EP 1092723 | A2 | 20010418 | EP 2000-308983 | 20001012 |
| EP 1092723 | A3 | 20010926 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO | | | | |
| JP 2001114792 | A | 20010424 | JP 1999-288952 | 19991012 |
| CA 2322936 | A1 | 20010412 | CA 2000-2322936 | 20001011 |
| US 6607710 | B1 | 20030819 | US 2000-686372 | 20001012 |
| PRIORITY APPLN. INFO.: | | | JP 1999-288952 | A 19991012 |

OTHER SOURCE(S): MARPAT 134:292147

AB An object of the present invention is to provide a bisphosphonic acid derivative and said bisphosphonic acid derivative being labeled with a radioactive nuclide, which has properties of rapid accumulation to the bone and rapid urinary excretion. The present invention relates to a bisphosphonic acid derivative and said bisphosphonic acid derivative being labeled with a radioactive nuclide, which is represented by the general formula R-Y-A, wherein A is a bisphosphonic acid or a salt thereof, having P-C-P bond; Y is a bonding portion such as a methylene, an amido etc.; R is a group of any one of a polyaminopolycarboxylic acid, an aliphatic carboxylic acid, a mercaptoacetylpolyamino acid or its derivs. and a disubstituted benzene compound where one substituent is a halogen atom or an isotope thereof or an alkyl tin; and the second substituent is a group of any one of compds. of an aminocarboxylic acid, an alkylocarboxylic acid or a substituted-alkylcarboxylic acid, an alkysulfonic acid or a substituted-alkysulfonic acid. The radiolabeled bisphosphonate derivative which has an affinity for bone can be used in diagnosis or therapy of bone diseases.

L4 ANSWER 12 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:581385 HCPLUS
 DOCUMENT NUMBER: 132:3542
 TITLE: Direct solid-phase synthesis of octreotide conjugates:
 precursors for use as tumor-targeted
 radiopharmaceuticals
 AUTHOR(S): Hsieh, H.-P.; Wu, Y.-T.; Chen, S.-T.; Wang, K.-T.
 CORPORATE SOURCE: Institute of Biological Chemistry, Academia Sinica,
 Nankang, Taiwan
 SOURCE: Bioorganic & Medicinal Chemistry (1999), 7(9),
 1797-1803
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Somatostatin analogs, such as octreotide, are useful for the visualization
 and treatment of tumors. Unfortunately, these compds. were produced
 synthetically using complex and inefficient procedures. Here, the authors
 describe a novel approach for the synthesis of octreotide and its analogs
 using p-carboxybenzaldehyde to anchor Fmoc-threoninol to solid phase
 resins. The reaction of the two hydroxyl groups of Fmoc-threoninol with
 p-carboxybenzaldehyde was catalyzed with p-toluenesulfonic acid in
 chloroform using a Dean-Stark apparatus to form Fmoc-threoninol
 p-carboxybenzacetal in 91% yield. The Fmoc-threoninol p-carboxybenzacetal
 acted as an Fmoc-amino acid derivative and the carboxyl group of
 Fmoc-threoninol p-carboxybenzacetal was coupled to an amine-resin via a
 DCC coupling reaction. The synthesis of protected octreotide and its
 conjugates were carried out in their entirety using a conventional Fmoc
 protocol and an autosynthesizer. The acetal was stable during the
 stepwise elongation of each Fmoc-amino acid as shown by the averaged
 coupling yield (>95%). Octreotide (74 to 78% yield) and five conjugated
 derivs. were synthesized with high yields using this procedure, including
 three radiotherapy octreotides (62 to 75% yield) and two cellular markers
 (72 to 76% yield). This novel approach provides a strategy for the rapid
 and efficient large-scale synthesis of octreotide and its analogs for
 radiopharmaceutical and tagged conjugates.

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:409606 HCPLUS
 DOCUMENT NUMBER: 131:56136
 TITLE: Dendritic polymer-saccharide conjugates and their
 preparation for use in NMR contrast media
 INVENTOR(S): Berndorff, Dietmar; Mareski, Peter; Misselwitz, Bernd;
 Platzek, Johannes; Raduechel, Bernd; Weinmann,
 Hanns-Joachim
 PATENT ASSIGNEE(S): Schering A.-G., Germany
 SOURCE: Ger. Offen., 54 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|-------|-----------------|-------|
| ----- | ---- | ----- | ----- | ----- |

| | | | | |
|--|----|----------|------------------|----------|
| DE 19758105 | A1 | 19990624 | DE 1997-19758105 | 19971218 |
| WO 9932154 | A1 | 19990701 | WO 1998-EP7927 | 19981209 |
| W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH,
GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK,
SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE | | | | |
| AU 9922680 | A | 19990712 | AU 1999-22680 | 19981209 |
| EP 1037672 | A1 | 20000927 | EP 1998-966256 | 19981209 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, FI | | | | |
| JP 2001526247 | T | 20011218 | JP 2000-525144 | 19981209 |
| PRIORITY APPLN. INFO.: DE 1997-19758105 A 19971218
WO 1998-EP7927 W 19981209 | | | | |
| AB The title conjugates, PKm(LZ)n (P = dendritic polymer with 12-150 amino groups; K = metal chelate group as detectable label; L = linker; Z = mono- or oligosaccharide group; m, n = 1-149), are excellent contrast agents for NMR diagnostics, especially for lymphog. These conjugates are accumulated by the lymphatic system adequately for imaging, in some cases even sufficiently for morphol. differentiation of lymph nodes. They are relatively nontoxic, are excreted slowly (>98% in 14 days), and show a high relaxivity which allows their use in low dosages. Thus, a dendritic polyamine with 64 amino groups, of which 38 bore Gd-DTPA chelate groups and 26 were substituted with 1-(4-thioureidophenyl)- α -D-mannopyranosyl groups, when injected i.v. at 200 μ mol Gd/kg into rats, was accumulated in the liver, spleen, and especially in the mesenteric and peripheral lymph nodes. Owing to the high relaxivity of this compound in water (17.0 L/mmol s), a dose of \geq 10 μ mol Gd/kg for i.v. NMR lymphog. is recommended. Preparation of this and other contrast agents from the unsubstituted dendritic polyamines is described. | | | | |

L4 ANSWER 14 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:53428 HCPLUS
 DOCUMENT NUMBER: 130:125343
 TITLE: Saccharide conjugates, their preparation and use as contrast agents and therapeutic agents
 INVENTOR(S): Mareski, Peter; Platzek, Johannes; Raduechel, Bernd;
 Berndorff, Dietmar; Weinmann, Hanns-Joachim
 PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
 SOURCE: PCT Int. Appl., 189 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|----------|
| WO 9901160 | A1 | 19990114 | WO 1998-EP3142 | 19980527 |
| W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH,
GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI,
SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE | | | | |
| DE 19728954 | C1 | 19990422 | DE 1997-19728954 | 19970630 |
| AU 9882109 | A | 19990125 | AU 1998-82109 | 19980527 |

PRIORITY APPLN. INFO.:

DE 1997-19728954

A 19970630

WO 1998-EP3142

W 19980527

AB Conjugates PKm(LZ)_n [P = polymer containing k amino groups; K = signal-generating chelating group containing metal ion; Z = mono- or Oligosaccharide; L = linker; m, n = 1-149; k = 12-150; (m + n) ≤ k], optionally addnl. containing cations of inorg. and/or organic bases, amino acids, or amino acid amides, are valuable compds. for diagnosis and therapy, especially for NMR lymphog. These compds. are accumulated by lymph nodes and the lymphatic system sufficiently for good imaging, are well tolerated, have a low excretion time (generally >98% elimination within 14 days) and a high relaxivity, show no species-specific aberrations, and frequently allow morphol. differentiation of lymph node tissue. For diagnostic NMR imaging, the metal ion is paramagnetic; for therapeutic use of the conjugates, the metal ion is radioactive. Thus, DTPA monoanhydride mono-Et ester reacted with poly-L-lysine-HBr in aqueous solution at pH 9.5 to form a conjugate with a degree of substitution (d.s.) of 58.7% (47 DTPA units/mol.). This conjugate reacted with p-isothiocyanatophenyl-β-D-galactopyranose to produce a glycosyl conjugate with d.s. 41.1% (33 galactosyl residues/mol.). The glycosyl conjugate reacted with GdCl₃ in aqueous buffer (pH 5.3) to produce the Gd chelate with no remaining free amino groups.

REFERENCE COUNT:

13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:642664 HCPLUS

DOCUMENT NUMBER: 130:10828

TITLE: Renal Metabolism of ¹¹¹In-DTPA-D-Phe1-Octreotide in Vivo

AUTHOR(S): Akizawa, Hiromichi; Arano, Yasushi; Uezono, Takashi; Ono, Masahiro; Fujioka, Yasushi; Uehara, Tomoya; Yokoyama, Akira; Akaji, Kenichi; Kiso, Yoshiaki; Koizumi, Mitsuru; Saji, Hideo

CORPORATE SOURCE: Department of Patho-Functional Bioanalysis Graduate School of Pharmaceutical Sciences, Kyoto University, Yoshida-Shimoadachi-cho Sakyo-ku Kyoto, 606-8501, Japan

SOURCE: Bioconjugate Chemistry (1998), 9(6), 662-670
CODEN: BCCHE; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The persistent localization of radioactivity in the kidney after administration of ¹¹¹In-DTPA-D-Phe1-octreotide impairs the diagnostic accuracy of this radiopharmaceutical. To better understand the mechanisms responsible for the renal radioactivity levels of ¹¹¹In-DTPA-D-Phe1-octreotide, the renal metabolism of this compound was compared with ¹¹¹In-DTPA-L-Phe1-octreotide, where the N-terminal D-phenylalanine was replaced with L-phenylalanine to facilitate metabolism. DTPA-D-Phe1-octreotide and DTPA-L-Phe1-octreotide were synthesized by solid-phase methods. Both ¹¹¹In-DTPA-conjugated octreotide analogs were prepared with radiochem. yields of over 96%, and both remained stable after a 3 h incubation in murine serum at 37°. When injected into mice, the two ¹¹¹In-DTPA-conjugated octreotide analogs showed similar radioactivity elimination rates from the blood and accumulation in the kidney with about 60% injected radioactivity being excreted in the urine by 24 h postinjection. Over 85% of the radioactivity in the urine existed as intact peptides for both analogs. Despite the similar renal radioactivity

levels, significant differences were observed in the radiolabeled species remaining in the kidney between the two; while ^{111}In -DTPA-L-Phe1-octreotide was rapidly metabolized to the final radiometabolite, ^{111}In -DTPA-L-Phe, the metabolic rate of ^{111}In -DTPA-D-Phe1-octreotide was so slow that various intermediate radiolabeled species were observed. However, both ^{111}In -DTPA-D-Phe and ^{111}In -DTPA-L-Phe remained in the lysosomal compartment of the renal cells as the final radiometabolites for long periods. These findings indicated that although the metabolic stability of ^{111}In -DTPA-D-Phe1-octreotide in the renal cells may be partially involved, the slow elimination rate of the radiometabolite derived from ^{111}In -DTPA-D-Phe1-octreotide from the lysosomal compartment of renal cells would be predominantly attributable to the persistent renal radioactivity levels of ^{111}In -DTPA-D-Phe1-octreotide.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:440582 HCPLUS

DOCUMENT NUMBER: 129:245447

TITLE: Synthesis of metabolically stabilized peptides and their radiolabeling: new $[^{111}\text{In}]$ - and $[^*\text{I}]$ -neurotensin analogs

AUTHOR(S): Tourwe, D.; Mertens, J.; Ceusters, M.; Jeannin, L.; Iterbeke, K.; Terriere, D.; Chavatte, C.; Boumon, R.

CORPORATE SOURCE: Organic Chemistry Department, Vrije Universiteit Brussel, Brussels, B-1050, Belg.

SOURCE: Tumor Targeting (1998), 3(1), 41-45
CODEN: TUTAF9; ISSN: 1351-8488

PUBLISHER: Stockton Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Neurotensin (NT) is a neuropeptide which binds with high affinity to receptors in various tumors: small cell lung carcinoma, human colon and pancreas carcinoma and meningiomas. Radiolabeled analogs are therefore potentially useful for diagnosis and therapy. Because of rapid metabolism *in vivo*, metabolically stabilized analogs have to be prepared. An approach is described based on the replacement of the scissile peptide bond by an isosteric $\psi[\text{CH}_2\text{NH}]$ function. For radioiodination using the Cu(I)-assisted nucleophilic exchange method, brominated benzoyl or phenylacetyl groups are attached to the N-terminus of NT(8-13). These retain high affinity for NT receptors and are radioiodinated with high radiochem. yield. For ^{111}In labeling, DTPA was attached to the N-terminus of NT(8-13) using a monoreactive DTPA-tetra-tert-Bu ester. Labeling was performed in a kit formulation or NCA tracer was obtained after semi-prep HPLC. High affinity binding to NT receptors in guinea pig brain and in HT29 human adenocarcinoma cells was observed. The stability in human plasma for $[^{111}\text{In}]$ DTPA-NT(8-13) was only 9.8 min, whereas that of the corresponding Lys8 $\psi[\text{CH}_2\text{NH}]$ Arg9 analog exceeds 250 min.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:532575 HCPLUS

DOCUMENT NUMBER: 127:135556

TITLE: Preparation of diaza-, triaza- and tetraazaalkane chelating agents for use as medicinal diagnostic and therapeutic agents

INVENTOR(S): Platzek, Johannes; Mareski, Peter; Niedballa, Ulrich;

PATENT ASSIGNEE(S): Raduechel, Bernd
 Schering A.-G., Germany
 SOURCE: Ger. Offen., 11 pp.
 CODEN: GWXXBX

DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|------------|
| DE 19601060 | A1 | 19970710 | DE 1996-19601060 | 19960104 |
| DE 19601060 | C2 | 20020425 | | |
| CA 2241825 | A1 | 19970717 | CA 1996-2241825 | 19961220 |
| CA 2241825 | C | 20050927 | | |
| WO 9725305 | A1 | 19970717 | WO 1996-DE2476 | 19961220 |
| W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS,
JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW,
MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG,
US, UZ, VN | | | | |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML,
MR, NE, SN, TD, TG | | | | |
| AU 9718703 | A | 19970801 | AU 1997-18703 | 19961220 |
| EP 871608 | A1 | 19981021 | EP 1996-946110 | 19961220 |
| EP 871608 | B1 | 20000405 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, FI | | | | |
| JP 2000502715 | T | 20000307 | JP 1997-524731 | 19961220 |
| JP 3993235 | B2 | 20071017 | | |
| AT 191456 | T | 20000415 | AT 1996-946110 | 19961220 |
| ES 2145517 | T3 | 20000701 | ES 1996-946110 | 19961220 |
| PT 871608 | T | 20000731 | PT 1996-946110 | 19961220 |
| US 6080785 | A | 20000627 | US 1998-101032 | 19980629 |
| NO 9803103 | A | 19980703 | NO 1998-3103 | 19980703 |
| NO 322888 | B1 | 20061218 | | |
| GR 3033822 | T3 | 20001031 | GR 2000-401522 | 20000629 |
| PRIORITY APPLN. INFO.: | | | DE 1996-19601060 | A 19960104 |
| | | | WO 1996-DE2476 | W 19961220 |

OTHER SOURCE(S): CASREACT 127:135556; MARPAT 127:135556

AB The title compds. A1NHCHR1CHR2(NA1CH2CH2)nNA12 and
 A1(A2)NCHR1CHR2(NA1CH2CH2)nNA12 [n = 0-2; A1 = CH2CO2CMe3; A2 = CH2CO2H;
 R1, R2 = H, or when n = 0 then R1R2 = (CH2)_m; m = 3-6], useful as
 antidotes for heavy metal poisoning (no data), MRI diagnostics (no data),
 radiog. diagnostics (no data), and agents for radiotherapy (no data), are
 prepared by the alkylation of a properly blocked azaalkane with tert-Bu or
 lower-alkyl-leaving-group haloacetate esters, followed by
 lower-alkyl-leaving-group ester hydrolysis and removal of relevant
 blocking groups. Thus, 1,4,7-triazaheptane was protected with Et
 trifluoroacetate, the intermediate alkylated with tert-Bu bromoacetate,
 hydrolyzed with NH4OH, alkylated with benzyl bromoacetate, and the
 intermediate hydrogenated, producing di-tert-Bu 6,9-bis(tert-
 butoxycarbonylmethyl)-3-carboxymethyl-3,6,9-triazaundecanedicarboxylate.

L4 ANSWER 18 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:299305 HCPLUS

DOCUMENT NUMBER: 126:317625

TITLE: Conventional and High-Yield Synthesis of

AUTHOR(S) : DTPA-Conjugated Peptides: Application of a Monoreactive DTPA to DTPA-D-Phe1-octreotide Synthesis
 Arano, Yasushi; Akizawa, Hiromichi; Uezono, Takashi;
 Akaji, Kenichi; Ono, Masahiro; Funakoshi, Susumu;
 Koizumi, Mitsuru; Yokoyama, Akira; Kiso, Yoshiaki;
 Saji, Hideo

CORPORATE SOURCE: Dep. Radiopharm. Chem., Kyoto Univ., Kyoto, 606-01,
 Japan

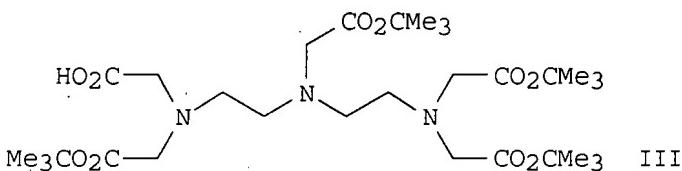
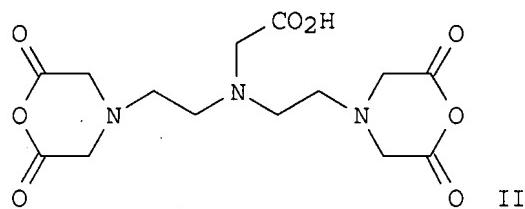
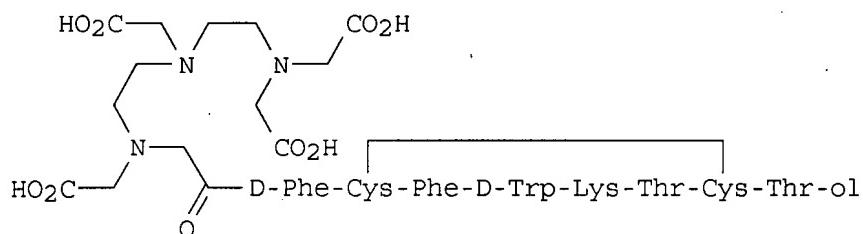
SOURCE: Bioconjugate Chemistry (1997), 8(3), 442-446
 CODEN: BCCHE; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Successful imaging of somatostatin receptor-pos. tumors with ^{111}In -DTPA-D-Phe1-octreotide (^{111}In -I) has stimulated development of peptide radiopharmaceuticals using DTPA as the chelating agent. However, use of cyclic DTPA dianhydride II resulted in low synthetic yields of DTPA-peptide by either solution or solid-phase syntheses. This paper reports a novel high-yield synthetic procedure for DTPA-D-Phe1-octreotide that is applicable to other peptides of interest using monoreactive DTPA derivative III. Monoreactive DTPA derivative III possesses one free terminal carboxylic acid along with four carboxylates protected with tert-Bu ester (mDTPA) was synthesized. N-9-Fluorenylmethoxycarbonyl-O-tert-butyl-L-threoninol (Fmoc-Thr(tBu)-ol), prepared from Fmoc-Thr(tBu)-OH, was loaded onto 2-chlorotriptyl chloride resin. After construction of the peptide chains by Fmoc chemical, mDTPA was coupled to the α amine group of the peptide on the resin in the presence of 1,3-diisopropylcarbodiimide and

1-hydroxybenzotriazole. Treatment of the mDTPA-peptide-resin with trifluoroacetic acid-thioanisole removed the protecting groups and liberated [Cys(Acm)2,7]-octreotide-D-Phe1-DTPA from the resin. Iodine oxidation of the DTPA-peptide, followed by the reversed-phase HPLC purification,

produced DTPA-D-Phe1-octreotide in overall 31.8% yield based on the starting Fmoc-Thr(tBu)-ol-resin. The final product gave a single peak on anal. HPLC, and amino acid anal. and mass spectrometry confirmed the integrity of the product. ¹¹¹In radiolabeling of the product provided ¹¹¹In-DTPA-D-Phe1-octreotide with >95% radiochem. yield, as confirmed by anal. reversed-phase HPLC, TLC, and CAE. These findings indicated that use of mDTPA during solid-phase peptide synthesis greatly increased the synthetic yield of DTPA-D-Phe1-octreotide, due to the absence of nonselective reactions that are unavoidable when cDTPA is used. These results also suggested that mDTPA would be a versatile reagent to introduce DTPA with high yield into peptides of interest.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:483602 HCPLUS

DOCUMENT NUMBER: 125:162256

TITLE: Reassessment of Diethylenetriaminepentaacetic Dianhydride (DTPA) as a Chelating Agent for Indium-111 Labeling of Polypeptides Using a Newly Synthesized Monoreactive DTPA Derivative

AUTHOR(S): Arano, Yasushi; Uezono, Takashi; Akizawa, Hiromichi; Ono, Masahiro; Wakisaka, Kouji; Nakayama, Morio; Sakahara, Harumi; Konishi, Junji; Yokoyama, Akira

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kyoto University, Kyoto, 606-01, Japan

SOURCE: Journal of Medicinal Chemistry (1996), 39(18), 3451-3460

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Previous studies on indium-111 (¹¹¹In) labeling of polypeptides and peptides using cyclic diethylenetriaminepentaacetic dianhydride (cDTPA) as a bifunctional chelating agent (BCA) have indicated that DTPA might be a useful BCA for ¹¹¹In labeling of polypeptides at high specific activities when DTPA can be incorporated without inducing intra- or intermol. crosslinking. To investigate this hypothesis, a monoreactive DTPA derivative with a maleimide group as the peptide binding site (MDTPA) was designed and synthesized. A monoclonal antibody (OST7, IgG1) was used as a model polypeptide, and conjugation of MDTPA with OST7, ¹¹¹In radiolabeling of MDTPA-OST7, and the stability of ¹¹¹In-MDTPA-OST7 were investigated using cDTPA and benzyl-EDTA derivs. as refs. SDS-PAGE anal. demonstrated that while cDTPA induced intramol. crosslinking, no such undesirable side reactions were observed with MDTPA. MDTPA generated ¹¹¹In-labeled OST7 with high radiochem. yields at higher specific activities than those produced using cDTPA and benzyl-EDTA derivs. as the BCAs. Incubation of each ¹¹¹In-labeled OST7 in human serum indicated that MDTPA generated ¹¹¹In-labeled OST7 of much higher and a little lower stability than those derived from cDTPA and benzyl-EDTA derivs., resp. These findings indicated that the low in vivo stability of cDTPA-conjugated antibody reported previously is not attributable to low stability of ¹¹¹In-DTPA but to formation of intramol. crosslinking during cDTPA conjugation reactions.

The present study also indicated that MDTPA and its precursor, the tetra-tert-Bu derivative of DTPA, would be useful BCAs for ^{111}In radiolabeling of polypeptides that have rapid blood clearance with high specific activities.

L4 ANSWER 20 OF 20 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:267995 HCPLUS
 DOCUMENT NUMBER: 124:305630
 TITLE: Dimeric DTPA derivatives and their metal complexes, pharmaceutical media containing these complexes, their use in der diagnostics and therapy and process for the preparation of the complexes and the media
 INVENTOR(S): Krause, Werner; Maier, Franz-Karl; Bauer, Michael; Press, Wolf-Ruediger; Schuhmann-Giampieri, Gabriele; Platzek, Johannes; Schmitt-Willich, Heribert
 PATENT ASSIGNEE(S): Schering A.-G., Germany
 SOURCE: Ger. Offen., 25 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| DE 4428874 | A1 | 19960222 | DE 1994-4428874 | 19940808 |
| US 5695737 | A | 19971209 | US 1995-476117 | 19950607 |
| CA 2197074 | A1 | 19960222 | CA 1995-2197074 | 19950808 |
| WO 9605167 | A1 | 19960222 | WO 1995-EP3142 | 19950808 |
| W: AU, BY, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, RU, SK, UA, US, VN | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| AU 9533433 | A | 19960307 | AU 1995-33433 | 19950808 |
| AU 695878 | B2 | 19980827 | | |
| ZA 9506650 | A | 19960319 | ZA 1995-6650 | 19950808 |
| EP 775104 | A1 | 19970528 | EP 1995-929815 | 19950808 |
| EP 775104 | B1 | 19990506 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| CN 1156442 | A | 19970806 | CN 1995-194571 | 19950808 |
| JP 10503777 | T | 19980407 | JP 1995-506999 | 19950808 |
| HU 77532 | A2 | 19980528 | HU 1997-370 | 19950808 |
| AT 179696 | T | 19990515 | AT 1995-929815 | 19950808 |
| ES 2134487 | T3 | 19991001 | ES 1995-929815 | 19950808 |
| FI 9700535 | A | 19970207 | FI 1997-535 | 19970207 |
| NO 9700602 | A | 19970210 | NO 1997-602 | 19970210 |

PRIORITY APPLN. INFO.: DE 1994-4428874 A 19940808
 WO 1995-EP3142 W 19950808

AB Dimeric diethylenetriaminepentaacetic acid derivs. and their metal complexes (Z = 21-32, 37-39, 42-51, and 57-83) were prepared. Contrast agents using these compds. were prepared for use in nuclear medicine.

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| FULL ESTIMATED COST | 61.80 | 235.46 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |

10/776470 Therapeutic n DiagnosticConjugates

| CA SUBSCRIBER PRICE | ENTRY | SESSION |
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10/776470 Therapeutic n DiagnosticConjugates

=> s 11

SAMPLE SEARCH INITIATED 17:13:10 FILE 'CASREACT'
SCREENING COMPLETE - 56 REACTIONS TO VERIFY FROM

7 DOCUMENTS

100.0% DONE 56 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 672 TO 1568
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L1 (0 REACTIONS)

=> s 11 sss full

FULL SEARCH INITIATED 17:13:31 FILE 'CASREACT'
SCREENING COMPLETE - 2593 REACTIONS TO VERIFY FROM 155 DOCUMENTS

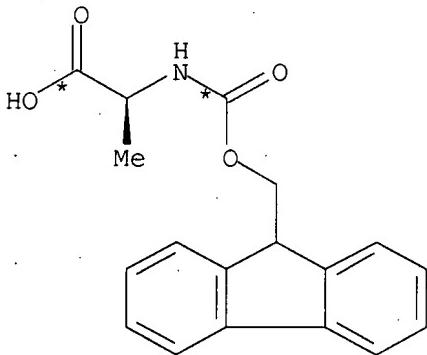
100.0% DONE 2593 VERIFIED 17 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.01

L6 3 SEA SSS FUL L1 (17 REACTIONS)

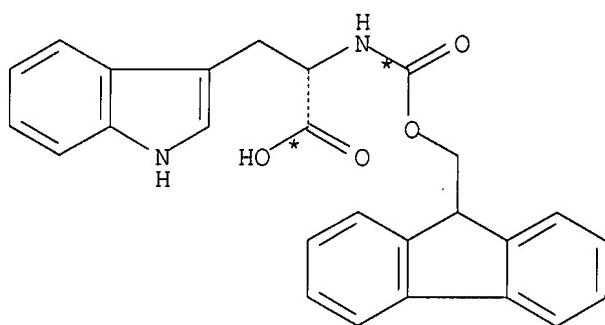
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L6 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

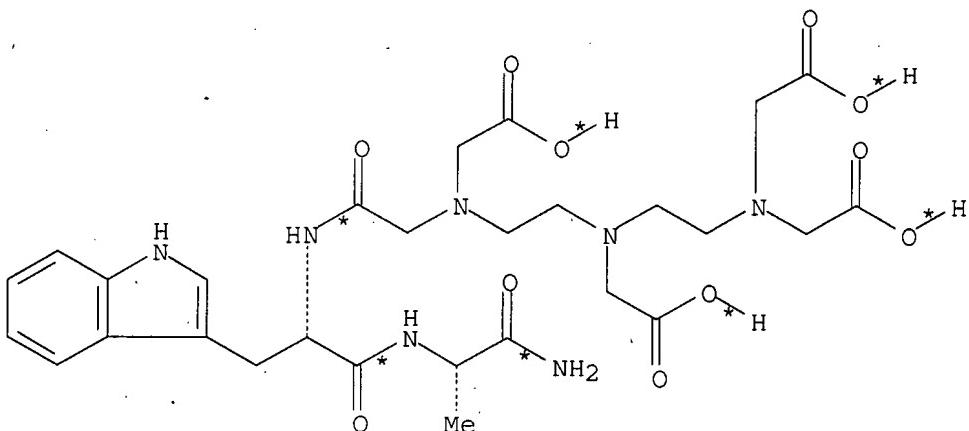
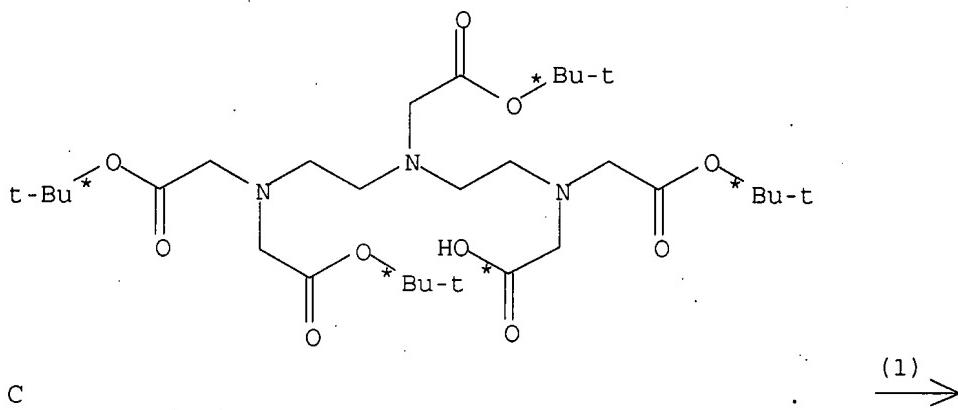
RX(1) OF 13 A + B + C ==> D



A



B



RX(1) RCT A 35661-39-3

STAGE(1)

RGT E 125700-67-6 Benzotriazolium der, F 7087-68-5 EtN(Pr-i)2,
G 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF
CON 1 - 3 hour, room temperature

STAGE(2)

RGT H 110-89-4 Piperidine
SOL 68-12-2 DMF
CON 15 - 30 minutes, room temperature

STAGE(3)

RCT B 35737-15-6
RGT E 125700-67-6 Benzotriazolium der, F 7087-68-5 EtN(Pr-i)2,
G 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF
CON 1 - 3 hour, room temperature

STAGE(4)

RGT H 110-89-4 Piperidine
 SOL 68-12-2 DMF
 CON 15 - 30 minutes, room temperature

STAGE(5)

RCT C 180152-83-4
 RGT E 125700-67-6 Benzotriazolium der, F 7087-68-5 EtN(Pr-i)2,
 G 2592-95-2 1-Benzotriazolol
 SOL 68-12-2 DMF
 CON 1 - 3 hour, room temperature

STAGE(6)

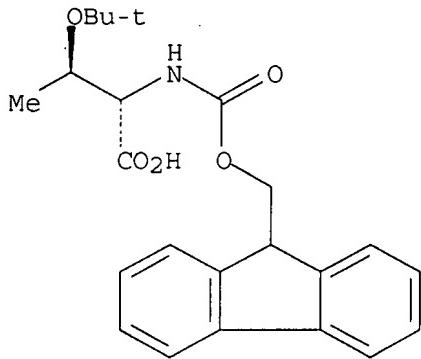
RGT I 6485-79-6 Silane, tris(1-methylethyl)-, J 76-05-1 F3CCO2H
 SOL 7732-18-5 Water
 CON 3 hours, room temperature

PRO D 899838-81-4

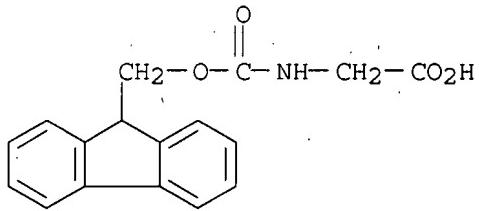
NTE solid-supported reaction, first stage attachment to Rink amide resin

L6 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

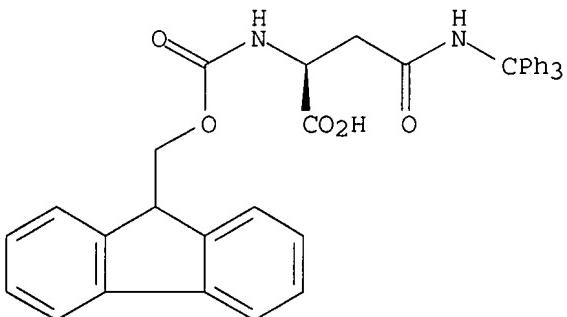
RX(1) OF 15 A + B + C + D + E + F ==> G...



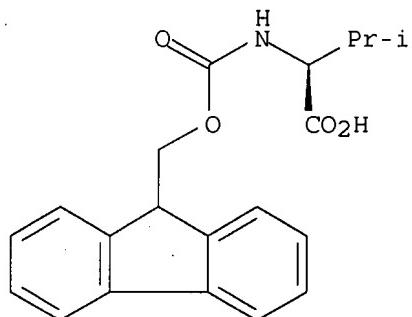
A



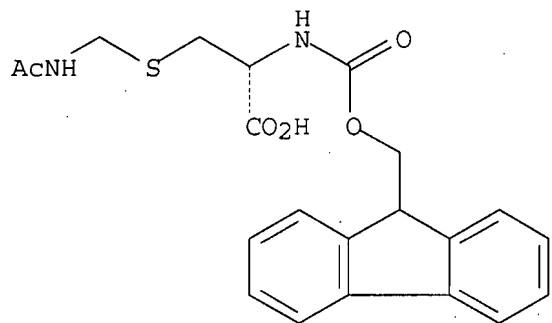
B



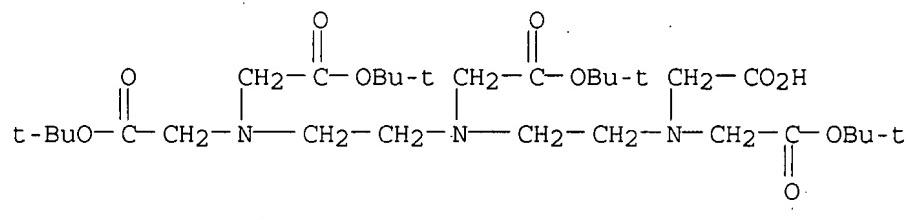
C



D



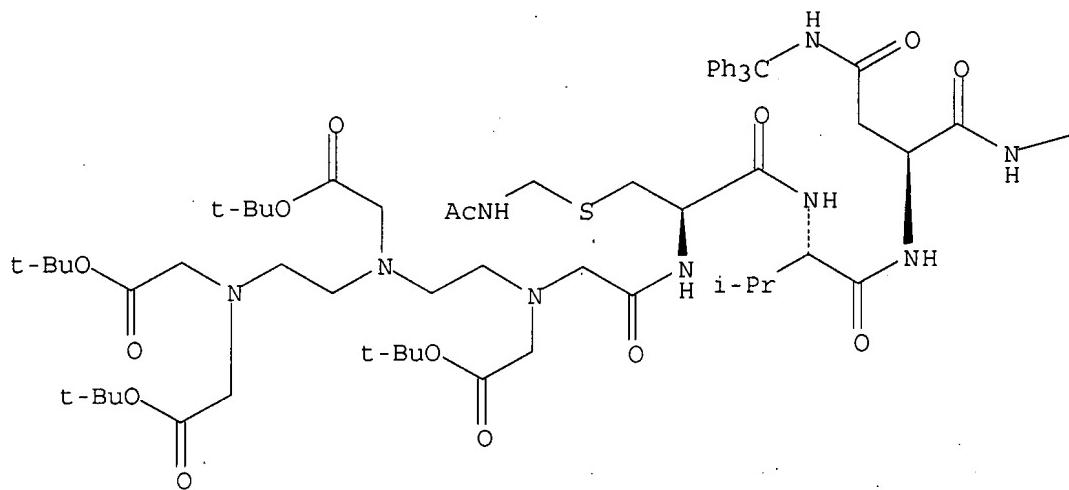
E

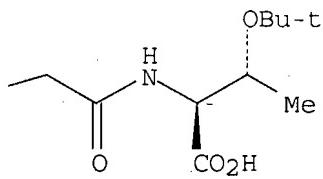


F

(1) →

PAGE 1-A





G

RX(1) RCT A 71989-35-0

STAGE(1)

STAGE(2)

RCT B 29022-11-5

STAGE(3)

RCT C 132388-59-1

STAGE(4)

RCT D 68858-20-8

STAGE(5)

RCT E 86060-81-3

STAGE(6)

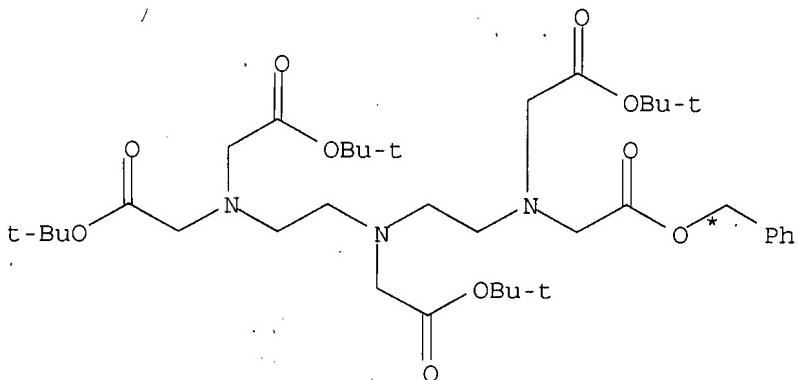
RCT F 180152-83-4

PRO G 796848-49-2

NTE no experimental detail, solid-supported reaction(first stage attachment to 2-chlorotritiy chloride resin)

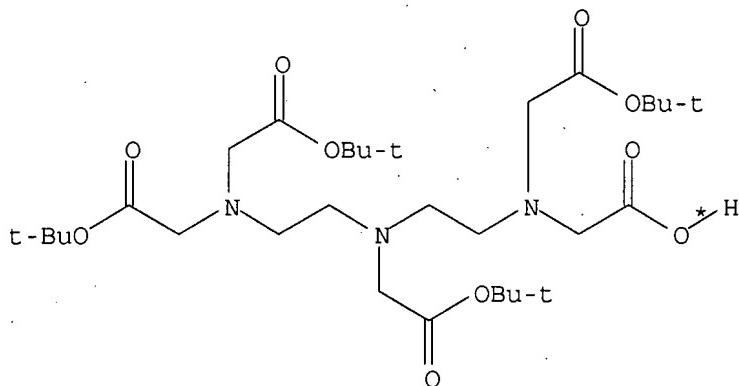
L6 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 2 A ==> B



A

(1) →



B
YIELD 96%

RX(1) RCT A 180152-87-8
PRO B 180152-83-4
SOL 67-63-0 Me2CHOH
NTE 0-40.deg., H2

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| => fil stng | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 121.17 | 357.95 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -15.60 |

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FILE CONTAINS CURRENT INFORMATION.
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| => fil stng | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 0.24 | 358.19 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -15.60 |

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Oct 26, 2007 (20071026/UP).

10/776470 Therapeutic n DiagnosticConjugates

| => file casreact | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | 0.06 | 358.25 |
| FULL ESTIMATED COST | | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -15.60 |

FILE 'CASREACT' ENTERED AT 17:17:07 ON 29 OCT 2007
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FILE CONTENT:1840 - 27 Oct 2007 VOL 147 ISS 19

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*
* .CASREACT now has more than 13.8 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 16:55:45 ON 29 OCT 2007)

FILE 'REGISTRY' ENTERED AT 16:55:55 ON 29 OCT 2007
L1 STRUCTURE uploaded
L2 1 S L1
L3 5 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 16:58:28 ON 29 OCT 2007
L4 20 S L3

FILE 'STNGUIDE' ENTERED AT 16:59:41 ON 29 OCT 2007

FILE 'CASREACT' ENTERED AT 17:13:04 ON 29 OCT 2007
L5 0 S L1
L6 3 S L1 SSS FULL

FILE 'STNGUIDE' ENTERED AT 17:14:52 ON 29 OCT 2007

FILE 'STNGUIDE' ENTERED AT 17:17:00 ON 29 OCT 2007

10/776470 Therapeutic n DiagnosticConjugates

FILE 'CASREACT' ENTERED AT 17:17:07 ON 29 OCT 2007

=> d 16 1-3 ibib abs

L6 ANSWER 1 OF 3 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 145:140459 CASREACT
TITLE: Phosphorylation State-Responsive Lanthanide Peptide Conjugates: A Luminescence Switch Based on Reversible Complex Reorganization
AUTHOR(S): Tremblay, Matthew S.; Zhu, Qing; Marti, Angel A.; Dyer, Joanne; Halim, Marlin; Jockusch, Steffen; Turro, Nicholas J.; Sames, Dalibor
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027; USA
SOURCE: Organic Letters (2006), 8(13), 2723-2726
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A luminogenic probe for peptide dephosphorylation has been developed. It consists of a serine-/tyrosine-containing peptide modified on the N-terminus with a tryptophan residue and a DTPA chelate capable of binding Tb³⁺. The authors propose a mechanistic model for the luminescence enhancement based on the interconversion of monomeric and dimeric lanthanide species, which is affected by the phosphorylation state of the serine or tyrosine residue. The optical switch reports effectively on phosphatase-catalyzed dephosphorylation in vitro.
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:421892 CASREACT
TITLE: De Novo Designed Peptidic Redox Potential Probe: Linking Sensitized Emission to Disulfide Bond Formation
AUTHOR(S): Lee, Kyung; Dzubeck, Valerie; Latshaw, Lauren; Schneider, Joel P.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716-2522, USA
SOURCE: Journal of the American Chemical Society (2004), 126(42), 13616-13617
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The design and utility of a peptidic probe capable of accurately measuring environmental redox potential via sensitized emission has been prepared. This probe is characterized by long-lived luminescence (millisecond), nanomolar detection limits, and a probe reduction potential of -0.243 V.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 127:135556 CASREACT
TITLE: Preparation of diaza-, triaza- and tetraazaalkane

chelating agents for use as medicinal diagnostic and therapeutic agents
 INVENTOR(S) : Platzek, Johannes; Mareski, Peter; Niedballa, Ulrich;
 Raduechel, Bernd
 PATENT ASSIGNEE(S) : Schering A.-G., Germany
 SOURCE: Ger. Offen., 11 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|----------|
| DE 19601060 | A1 | 19970710 | DE 1996-19601060 | 19960104 |
| DE 19601060 | C2 | 20020425 | | |
| CA 2241825 | A1 | 19970717 | CA 1996-2241825 | 19961220 |
| CA 2241825 | C | 20050927 | | |
| WO 9725305 | A1 | 19970717 | WO 1996-DE2476 | 19961220 |
| W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IL, IS,
JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW,
MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG,
US, UZ, VN | | | | |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML,
MR, NE, SN, TD, TG | | | | |
| AU 9718703 | A | 19970801 | AU 1997-18703 | 19961220 |
| EP 871608 | A1 | 19981021 | EP 1996-946110 | 19961220 |
| EP 871608 | B1 | 20000405 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, FI | | | | |
| JP 2000502715 | T | 20000307 | JP 1997-524731 | 19961220 |
| JP 3993235 | B2 | 20071017 | | |
| AT 191456 | T | 20000415 | AT 1996-946110 | 19961220 |
| ES 2145517 | T3 | 20000701 | ES 1996-946110 | 19961220 |
| PT 871608 | T | 20000731 | PT 1996-946110 | 19961220 |
| US 6080785 | A | 20000627 | US 1998-101032 | 19980629 |
| NO 9803103 | A | 19980703 | NO 1998-3103 | 19980703 |
| NO 322888 | B1 | 20061218 | | |
| GR 3033822 | T3 | 20001031 | GR 2000-401522 | 20000629 |
| PRIORITY APPLN. INFO.: | | | DE 1996-19601060 | 19960104 |
| | | | WO 1996-DE2476 | 19961220 |

OTHER SOURCE(S) : MARPAT 127:135556
 AB The title compds. A1NHCHR1CHR2(NA1CH2CH2)nNA12 and
 A1(A2)NCHR1CHR2(NA1CH2CH2)nNA12 [n = 0-2; A1 = CH2CO2CMe3; A2 = CH2CO2H;
 R1, R2 = H, or when n = 0 then R1R2 = (CH2)_m; m = 3-6], useful as
 antidotes for heavy metal poisoning (no data), MRI diagnostics (no data),
 radiog. diagnostics (no data), and agents for radiotherapy (no data), are
 prepared by the alkylation of a properly blocked azaalkane with tert-Bu or
 lower-alkyl-leaving-group haloacetate esters, followed by
 lower-alkyl-leaving-group ester hydrolysis and removal of relevant
 blocking groups. Thus, 1,4,7-triazaheptane was protected with Et
 trifluoroacetate, the intermediate alkylated with tert-Bu bromoacetate,
 hydrolyzed with NH4OH, alkylated with benzyl bromoacetate, and the
 intermediate hydrogenated, producing di-tert-Bu 6,9-bis(tert-
 butoxycarbonylmethyl)-3-carboxymethyl-3,6,9-triazaundecanedicarboxylate.

10/776470 Therapeutic n DiagnosticConjugates

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| => file stng | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 8.49 | 366.74 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -2.19 | -17.79 |

FILE 'STNGUIDE' ENTERED AT 17:17:58 ON 29 OCT 2007
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| | | |
|--|------------------|---------------|
| => file casreact | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 0.42 | 367.16 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -17.79 |

FILE 'CASREACT' ENTERED AT 17:22:03 ON 29 OCT 2007
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FILE CONTENT:1840 - 27 Oct 2007 VOL 147 ISS 19

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l1/pro
QUALIFICATION NOT VALID FOR L1
Field code qualifications can only be applied to text terms.

=> d his

10/776470 Therapeutic n DiagnosticConjugates

(FILE 'HOME' ENTERED AT 16:55:45 ON 29 OCT 2007)

FILE 'REGISTRY' ENTERED AT 16:55:55 ON 29 OCT 2007

L1 STRUCTURE UPLOADED
L2 1 S L1
L3 5 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 16:58:28 ON 29 OCT 2007

L4 20 S L3

FILE 'STNGUIDE' ENTERED AT 16:59:41 ON 29 OCT 2007

FILE 'CASREACT' ENTERED AT 17:13:04 ON 29 OCT 2007

L5 0 S L1
L6 3 S L1 SSS FULL

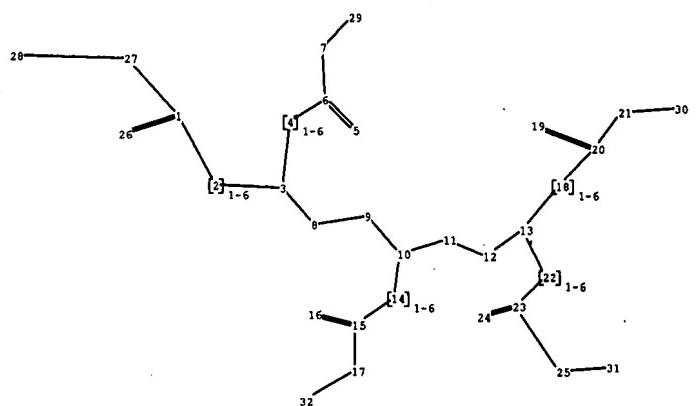
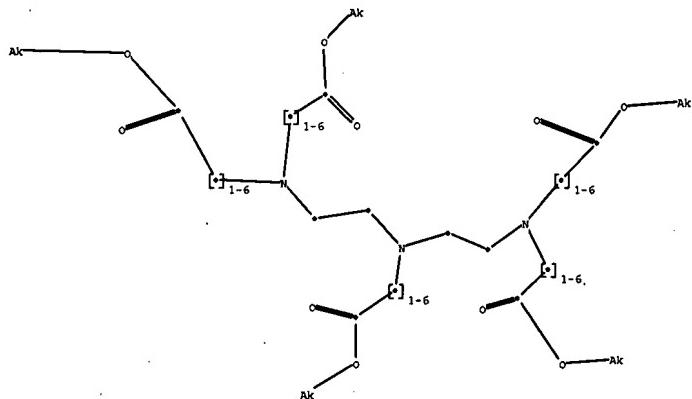
FILE 'STNGUIDE' ENTERED AT 17:14:52 ON 29 OCT 2007

FILE 'STNGUIDE' ENTERED AT 17:17:00 ON 29 OCT 2007

FILE 'CASREACT' ENTERED AT 17:17:07 ON 29 OCT 2007

FILE 'STNGUIDE' ENTERED AT 17:17:58 ON 29 OCT 2007

FILE 'CASREACT' ENTERED AT 17:22:03 ON 29 OCT 2007



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28
29 30 31 32

chain bonds :

1-2 1-26 1-27 2-3 3-4 3-8 4-6 5-6 6-7 7-29 8-9 9-10 10-11 10-14 11-12 12-13 13-18
13-22 14-15 15-16 15-17 17-32 18-20 19-20 20-21 21-30 22-23 23-24 23-25 25-31 27-28

exact/norm bonds :

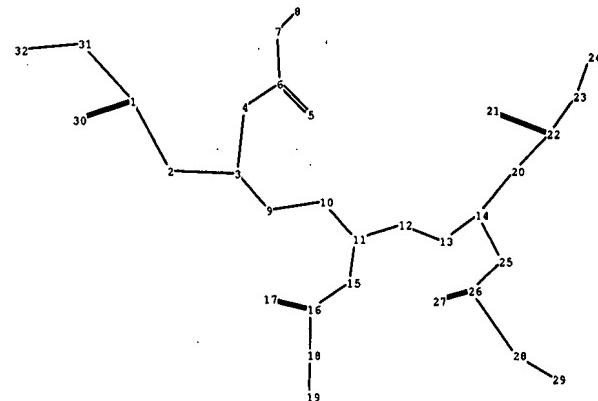
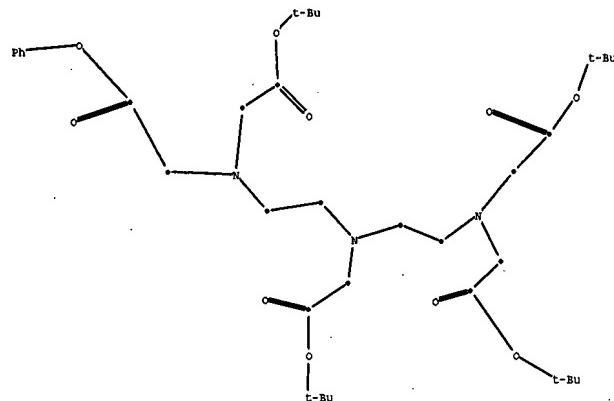
1-26 1-27 2-3 3-4 3-8 5-6 6-7 7-29 9-10 10-11 10-14 12-13 13-18 13-22 15-16 15-17
17-32 19-20 20-21 21-30 23-24 23-25 25-31 27-28

exact bonds :

1-2 4-6 8-9 11-12 14-15 18-20 22-23

Match level :

1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS
12:CLASS13:CLASS14:CLASS15:CLASS16:CLASS17:CLASS18:CLASS19:CLASS20:CLASS21:CLASS
22:CLASS23:CLASS24:CLASS25:CLASS26:CLASS27:CLASS28:CLASS29:CLASS30:CLASS31:CLASS
32:CLASS



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28
29 30 31 32

chain bonds :

1-2 1-30 1-31 2-3 3-4 3-9 4-6 5-6 6-7 7-8 9-10 10-11 11-12 11-15 12-13 13-14 14-20
14-25 15-16 16-17 16-18 18-19 20-22 21-22 22-23 23-24 25-26 26-27 26-28 28-29 31-32

exact/norm bonds :

1-30 1-31 2-3 3-4 3-9 5-6 6-7 10-11 11-12 11-15 13-14 14-20 14-25 16-17 16-18 21-22
22-23 26-27 26-28

exact bonds :

1-2 4-6 7-8 9-10 12-13 15-16 18-19 20-22 23-24 25-26 28-29 31-32

Match level :

1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS
12:CLASS13:CLASS14:CLASS15:CLASS16:CLASS17:CLASS18:CLASS19:CLASS20:CLASS21:CLASS
22:CLASS23:CLASS24:CLASS25:CLASS26:CLASS27:CLASS28:CLASS29:CLASS30:CLASS31:CLASS
32:CLASS